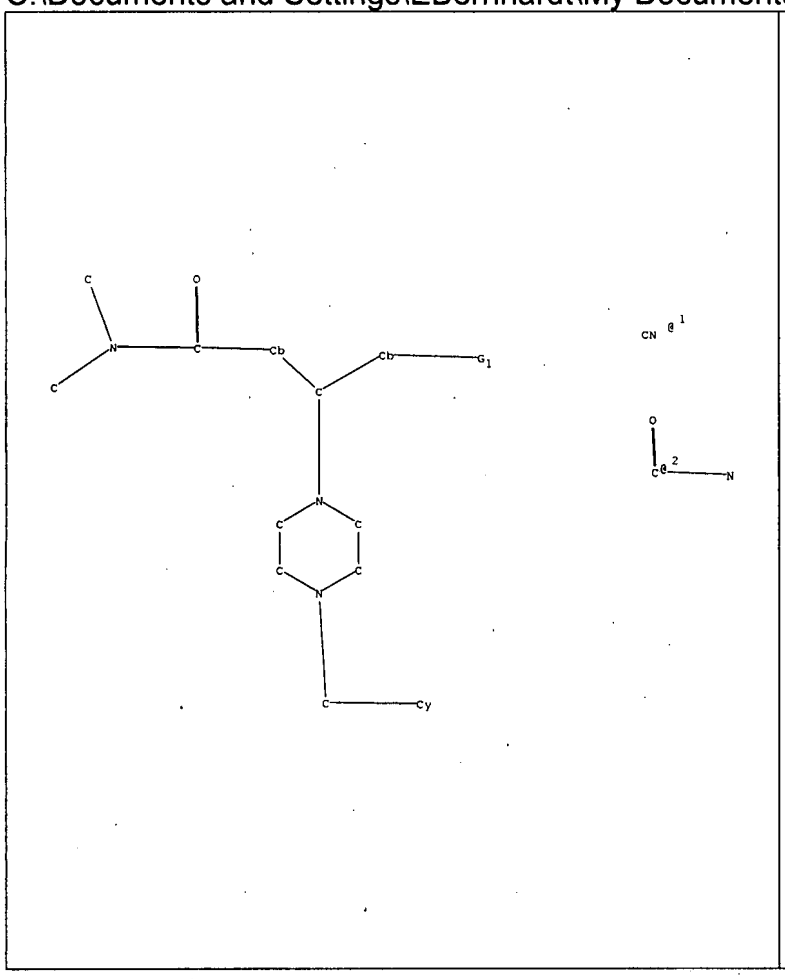
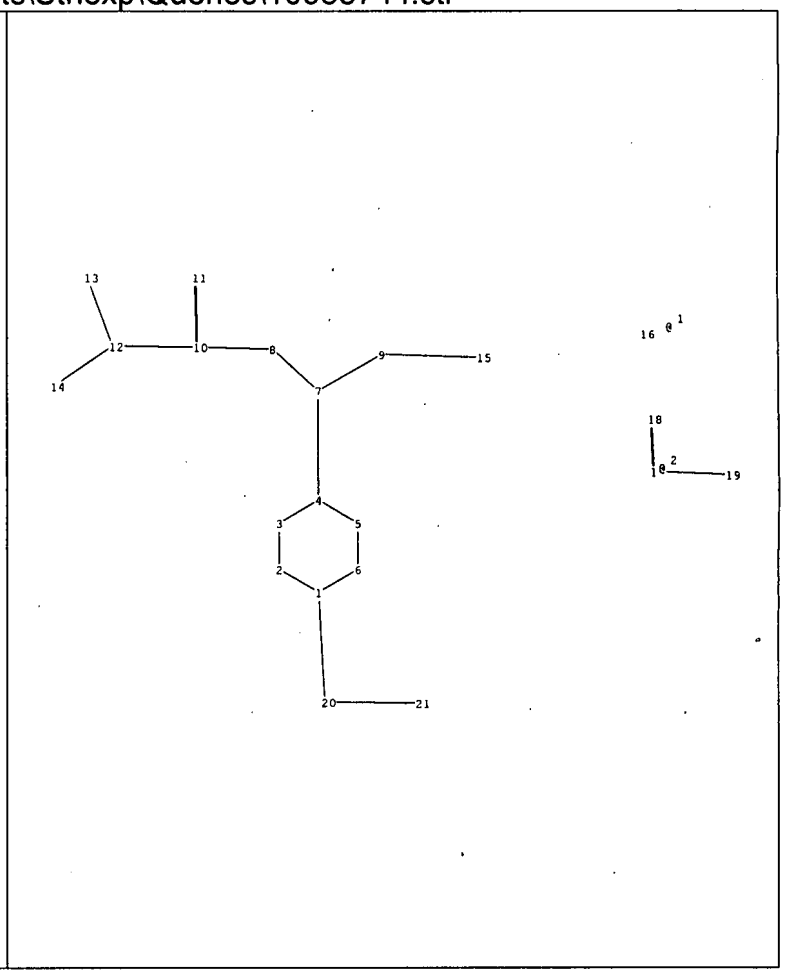
EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L4	454866	($3amino)carbonyl near2 phenyl near10 piperazin-1-yl	US-PGPUB; USPAT	OR	OFF	2007/06/23 18:52
L5	4819	((544/360) or (544/363) or (544/369) or (544/370) or (544/372) or (544/379) or (544/396)).CCLS.	US-PGPUB; USPAT	OR	OFF	2007/06/23 18:53
L7	3584	l4 and l5	US-PGPUB; USPAT	OR	OFF	2007/06/23 18:55
L8	1885	l7 and (opioid or sigma or delta)	US-PGPUB; USPAT	OR	OFF	2007/06/23 18:56

C:\Documents and Settings\EBernhardt\My Documents\Stnexp\Queries\10533744.str





chain nodes :
7 8 9 10 11 12 13 14 15 16 17 18 19 20 21
ring nodes :
1 2 3 4 5 6
chain bonds :
1-20 4-7 7-8 7-9 8-10 9-15 10-11 10-12 12-13 12-14 17-18 17-19 20-21
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 1-20 2-3 3-4 4-5 4-7 5-6 9-15 10-11 10-12 12-13 12-14 17-18 17-19 20-21
exact bonds :
7-8 7-9 8-10
isolated ring systems :
containing 1 :

G1:[*1],[*2]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:Atom
Generic attributes :
8:
Saturation : Unsaturated

Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
9:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
21:
Saturation : Unsaturated

```
=> d his

     (FILE 'HOME' ENTERED AT 16:03:26 ON 23 JUN 2007)

     FILE 'REGISTRY' ENTERED AT 16:03:42 ON 23 JUN 2007
L1             STRUCTURE UPLOADED
L2           0 S L1
L3          17 S L1 SSS FULL

     FILE 'CAPLUS' ENTERED AT 16:04:30 ON 23 JUN 2007
L4           1 S L3

     FILE 'CAOLD' ENTERED AT 16:04:59 ON 23 JUN 2007
L5           0 S L3

     FILE 'CHEMCATS' ENTERED AT 16:05:09 ON 23 JUN 2007
L6           0 S L3

     FILE 'REGISTRY' ENTERED AT 16:05:58 ON 23 JUN 2007

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                 0.45     178.23

FILE 'CAPLUS' ENTERED AT 16:06:29 ON 23 JUN 2007
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FILE LAST UPDATED: 22 Jun 2007  (20070622/ED)

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     (FILE 'HOME' ENTERED AT 16:03:26 ON 23 JUN 2007)

     FILE 'REGISTRY' ENTERED AT 16:03:42 ON 23 JUN 2007
L1             STRUCTURE UPLOADED
L2           0 S L1
L3          17 S L1 SSS FULL

     FILE 'CAPLUS' ENTERED AT 16:04:30 ON 23 JUN 2007
L4           1 S L3
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     FILE 'CAOLD' ENTERED AT 16:04:59 ON 23 JUN 2007
L5             0 S L3

     FILE 'CHEMCATS' ENTERED AT 16:05:09 ON 23 JUN 2007
L6             0 S L3

     FILE 'REGISTRY' ENTERED AT 16:05:58 ON 23 JUN 2007

     FILE 'CAPLUS' ENTERED AT 16:06:29 ON 23 JUN 2007

=> s l3 bib abs hitstr
MISSING OPERATOR L3 BIB
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> s l3
L7             1 L3

=> d l7 bib abs hitstr

L7   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2007 ACS on STN
AN   2004:412930  CAPLUS
DN   140:423707
TI   Preparation of 4-(phenylpiperazinylmethyl)benzamides for treatment of pain
     or gastrointestinal disorders
IN   Brown, William; Griffin, Andrew; Plobeck, Niklas; Walpole, Christopher
PA   Astrazeneca AB, Swed.
SO   PCT Int. Appl., 45 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.          DATE
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PI   WO 2004041800        A1     20040521    WO 2003-SE1703           20031105
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             GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
             OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
             TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2502733          A1     20040521    CA 2003-2502733          20031105
     AU 2003274884       A1     20040607    AU 2003-274884           20031105
     EP 1562922          A1     20050817    EP 2003-759164           20031105
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             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     BR 2003015998       A      20050920    BR 2003-15998            20031105
     CN 1711251          A      20051221    CN 2003-80102825         20031105
     JP 2006507296       T      20060302    JP 2004-549772           20031105
     US 2006167004       A1     20060727    US 2005-533744           20050504
     NO 2005002699       A      20050606    NO 2005-2699             20050606
PRAI SE 2002-3300        A      20021107
     WO 2003-SE1703      W      20031105
OS   MARPAT 140:423707
GI
```

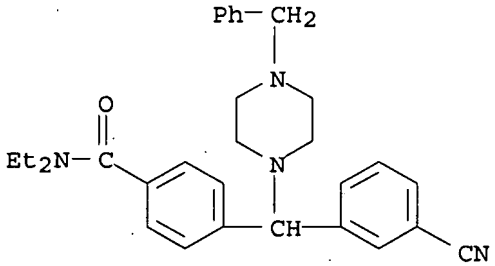
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [wherein R1 = (un)substituted (hetero)aryl; R2 = H or (un)substituted alkyl, aryl, or heterocyclyl; or pharmaceutically acceptable salts, enantiomers, or mixts. thereof] were prepared as opioid δ receptor ligands. For example, 4-carboxybenzaldehyde was amidated with diethylamine using SOCl2 in CH2Cl2 to give N,N-diethyl-4-formylbenzamide (90%). Coupling of the amide with 1-piperazinecarboxylic acid 1,1-dimethylethyl ester in the presence of benzotriazole in toluene, followed by reaction with 3-cyanophenylzinc iodide in THF, afforded 4-[(3-cyanophenyl)[4-[(diethylamino)carbonyl]phenyl]methyl]-1-piperazinecarboxylic acid 1,1-dimethylethyl ester. Deprotection of the piperazine (39%) using TFA in CH2Cl2 and alkylation (57%) with benzaldehyde in the presence of sodium triacetoxyborohydride in CH2Cl2 provided 3-[[4-[(diethylamino)carbonyl]phenyl](4-benzylpiperazin-1-yl)methyl]benzonitrile. Conversion of the nitrile to the amide with KOH in t-BuOH and chiral HPLC separation of the enantiomers gave (-)-II (99% optical purity). In binding assays using human 293S cells expressing cloned human opioid receptors and neomycin resistance, (-)-II proved to be an effective δ receptor ligand (IC50 = 0.26 nM) and showed some activity toward the κ (IC50 = 112 nM) and μ (IC50 = 7.7 nM) receptors. In functional assays, (-)-II demonstrated δ receptor agonist activity by activating the binding of GTP to G-proteins. Thus, I and their pharmaceutical compns. are useful in therapy, in particular for the treatment of gastrointestinal disorders or the management of pain (no data).

IT 691358-45-9P, 3-[[4-[(Diethylamino)carbonyl]phenyl](4-benzylpiperazin-1-yl)methyl]benzonitrile 691358-46-0P, 3-[[4-[(Diethylamino)carbonyl]phenyl][4-(2-furylmethyl)piperazin-1-yl]methyl]benzonitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of (phenylpiperazinylmethyl)benzamides as δ receptor agonists for treatment of pain or gastrointestinal disorders)

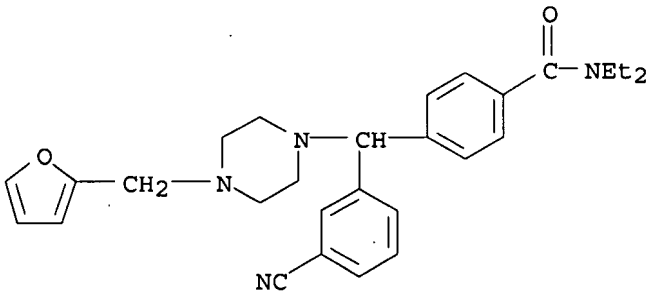
RN 691358-45-9 CAPLUS

CN Benzamide, 4-[(3-cyanophenyl)[4-(phenylmethyl)-1-piperazinyl]methyl]-N,N-diethyl- (9CI) (CA INDEX NAME)



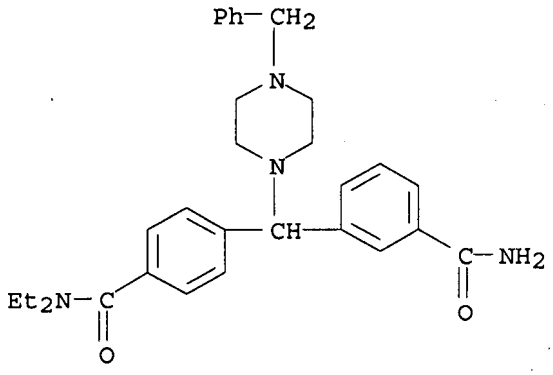
RN 691358-46-0 CAPLUS

CN Benzamide, 4-[(3-cyanophenyl)[4-(2-furanylmethyl)-1-piperazinyl]methyl]-N,N-diethyl- (9CI) (CA INDEX NAME)

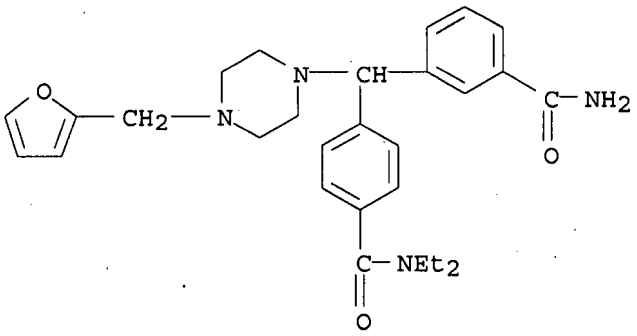


IT 691358-51-7P, 3-[[4-[(Diethylamino)carbonyl]phenyl](4-benzylpiperazin-1-yl)methyl]benzamide 691358-56-2P, 3-[[4-[(Diethylamino)carbonyl]phenyl][4-(2-furylmethyl)piperazin-1-yl]methyl]benzamide 691358-62-0P, 3-[[4-[(Diethylamino)carbonyl]phenyl][4-(phenylmethyl)-1-piperazinyl]methyl]-N-methylbenzamide
RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(δ receptor agonist; preparation of (phenylpiperazinylmethyl)benzamides as δ receptor agonists for treatment of pain or gastrointestinal disorders)

RN 691358-51-7 CAPLUS
CN Benzamide, 4-[[3-(aminocarbonyl)phenyl][4-(phenylmethyl)-1-piperazinyl]methyl]-N,N-diethyl- (9CI) (CA INDEX NAME)



RN 691358-56-2 CAPLUS
CN Benzamide, 4-[[3-(aminocarbonyl)phenyl][4-(2-furanylmethyl)-1-piperazinyl]methyl]-N,N-diethyl- (9CI) (CA INDEX NAME)



RN 691358-62-0 CAPLUS
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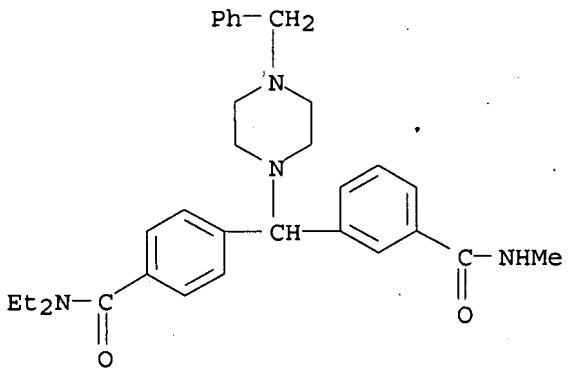
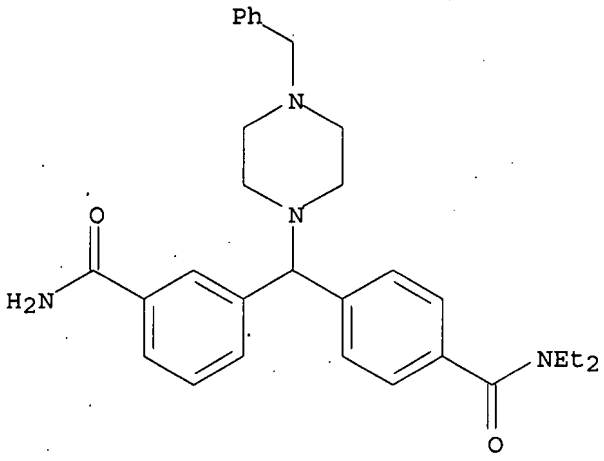


IT 691883-84-8P 691883-85-9P 691883-86-0P
691883-87-1P 691883-88-2P 691883-89-3P
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(δ receptor agonist; preparation of (phenylpiperazinylmethyl)benzamides as δ receptor agonists for treatment of pain or gastrointestinal disorders)
RN 691883-84-8 CAPLUS
CN Benzamide, 4-[[3-(aminocarbonyl)phenyl][4-(phenylmethyl)-1-piperazinyl]methyl]-N,N-diethyl-, hydrochloride (5:16), (-)- (9CI) (CA INDEX NAME)

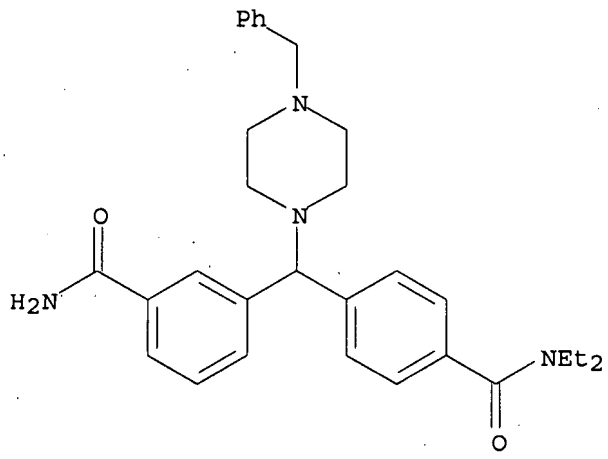
Rotation (-).



●16/5 HCl

RN 691883-85-9 CAPLUS
CN Benzamide, 4-[[3-(aminocarbonyl)phenyl][4-(phenylmethyl)-1-piperazinyl]methyl]-N,N-diethyl-, hydrochloride (10:31), (+)- (9CI) (CA INDEX NAME)

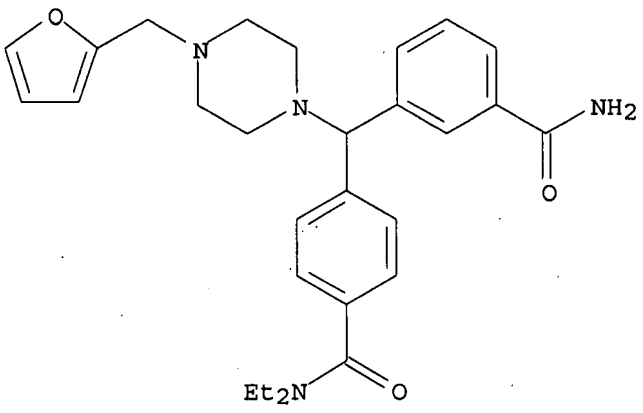
Rotation (+).



●31/10 HCl

RN 691883-86-0 CAPLUS
CN Benzamide, 4-[[3-(aminocarbonyl)phenyl][4-(2-furanylmethyl)-1-piperazinyl]methyl]-N,N-diethyl-, hydrochloride (5:13), (-)- (9CI) (CA INDEX NAME)

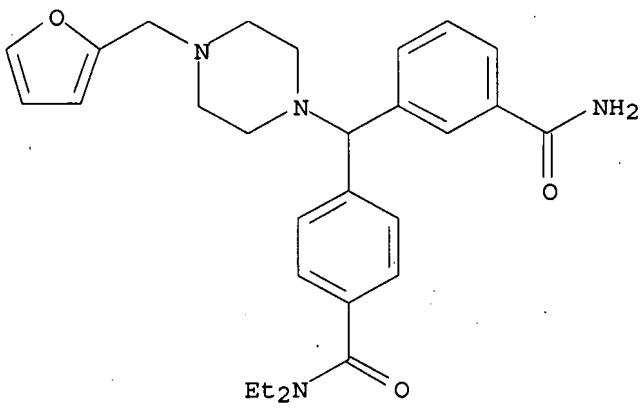
Rotation (-).



●13/5 HCl

RN 691883-87-1 CAPLUS
CN Benzamide, 4-[[3-(aminocarbonyl)phenyl][4-(2-furanylmethyl)-1-piperazinyl]methyl]-N,N-diethyl-, hydrochloride (10:7), (+)- (9CI) (CA INDEX NAME)

Rotation (+).



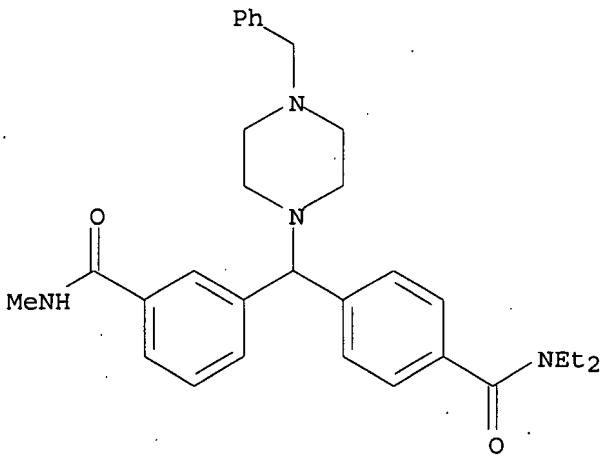
●7/10 HCl

RN 691883-88-2 CAPLUS
CN Benzamide, N,N-diethyl-4-[[3-[(methylamino)carbonyl]phenyl][4-(phenylmethyl)-1-piperazinyl]methyl]-, (-)-, trifluoroacetate (5:8) (9CI) (CA INDEX NAME)

CM 1

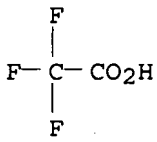
CRN 691358-63-1
CMF C31 H38 N4 O2

Rotation (-).



CM 2

CRN 76-05-1
CMF C2 H F3 O2

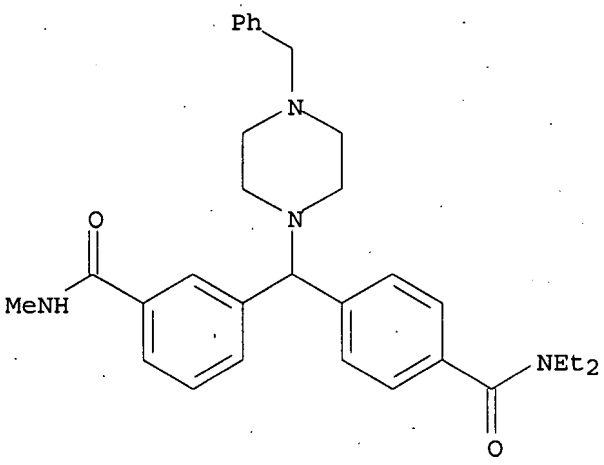


RN 691883-89-3 CAPLUS
CN Benzamide, N,N-diethyl-4-[[3-[(methylamino)carbonyl]phenyl][4-(phenylmethyl)-1-piperazinyl]methyl]-, (+)-, trifluoroacetate (5:8) (9CI) (CA INDEX NAME)

CM 1

CRN 691358-64-2
CMF C31 H38 N4 O2

Rotation (+).



CM 2

CRN 76-05-1
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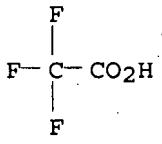

=> log h

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.74	183.97

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.78	-0.78

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 16:07:07 ON 23 JUN 2007